

# SINGULAR POTENTIALS AND ABSORPTION PROBLEM IN QUANTUM MECHANICS

VLADIMIR D. SKARZHINSKY<sup>1,2</sup> AND JÜRGEN AUDRETSCH<sup>2</sup>

<sup>1</sup> *P. N. Lebedev Physical Institute, Leninsky prospect 53, Moscow 117924, Russia,*

<sup>2</sup> *Fakultät für Physik der Universität Konstanz, Postfach M 673,  
D-78457 Konstanz, Germany*

We discuss a possible approach to the absorption problem in Quantum Mechanics based on using of singular attractive potentials in the corresponding Schrödinger equations. Possible criteria for selection of exact solutions of these equations are considered and it is shown that different models of absorption can be realized by a special choice of exact solutions. As an example, the motion of charged particles in the Aharonov-Bohm (AB) and the scalar attractive  $\rho^{-2}$  potentials is investigated in detail. Other attractive potentials are briefly considered.

## 1 Introduction

The introduction of complex potentials is generally accepted way to describe absorption at quantum scattering [1]. Based on an analogy with electrodynamics this method can be, nevertheless, disputed in QM because of quite different nature of wave functions and electromagnetic field. Proposed recently approach to the absorption using restricted Feynman-type integrals [2] seems to be more adequate to this problem. Also, absorption can be treated in connection with the well-known problem of collapse of particles scattered by singular potentials [3]. In contrast to the case of regular potentials the scattering by singular potentials leads to two linear independent solutions of radial Schrödinger equations that are both square-integrable and form overfull nonorthogonal set. This means that corresponding Hamiltonians are not self-adjoint. To describe elastic scattering the procedure of self-adjoint extension [4] has been applied by imposing suitable boundary conditions at singularity points. For the case of the singular attractive potential  $\sim r^{-n}$ ,  $n \geq 2$  they have been found in [5].

On the contrary, to describe absorption one has to refuse from the self-adjointness and permit non-hermitean Hamiltonians. They have been first employed with this aim in [6] where the capture of ions by polarization forces in  $\sim r^{-4}$ -potential was considered. Such interpretation of the collapse problem

has been developed in [7, 8] for the case of the singular attractive potentials  $\sim r^{-n}$ ,  $n \geq 2$ .

The absorption problem became practically important in last years in connection with atom interferometer experiments on scattering neutral polarizable atoms by a charge wire [9] as well as with superimposed magnetic field with the aim to observe the effect of the AB topological phase on this process. These processes are effectively governed by the Schrödinger equation with the AB - and the attractive  $\rho^{-2}$  potential in two dimensions. This unexpected application of the AB effect [10] in atomic physics [11, 12] has been recently discussed theoretically [13, 14, 15]. Absorption of atoms was an essential part of these investigations, and the corresponding atom interferometer experiment is on its way.

## 2 Absorption and inelastic scattering in the singular AB- and $\rho^{-2}$ potentials

The radial wave function for scattered particles with mass  $M$  and charge  $e$  in the AB-potential  $A_\varphi = \beta/\rho$ ,  $\beta$  being the magnetic flux in the m.f.q.units,  $0 \leq \beta < 1$ , and in a scalar potential  $U = -\kappa^2/\rho^2$  satisfies the Bessel equation

$$R_m''(\rho) + \frac{1}{\rho} R_m'(\rho) - \frac{\nu^2}{\rho^2} R_m(\rho) + p^2 R_m(\rho) = 0 \quad (1)$$

$$\nu^2 := (m - \beta)^2 - \gamma^2, \quad \gamma^2 := 2M\kappa^2. \quad (2)$$

The parameter  $\nu^2$  can be negative.

The differential operator Eq. (1) is *symmetric* but is not *self-adjoint*. Its self-adjoint extension depends on infinite number of *open parameters* [16]. Unfortunately, it has been not answered there of what type of physical situations corresponds in some limit to given values of open parameters. This turned out to be possible only for the pure AB case [17].

The partial scattering amplitudes  $f_m$  are expressed [14] in terms of phase shifts  $\delta_m$

$$f_m = \frac{e^{-i\frac{\pi}{4}}}{\sqrt{p}} (S_m - \cos \beta), \quad S_m := e^{2i\delta_m}. \quad (3)$$

which are defined by the asymptotic form of the radial functions

$$R_m(\rho) \rightarrow \sqrt{\frac{1}{2\pi p \rho}} \left[ e^{-i(p\rho - \pi m - \frac{\pi}{4})} + S_m e^{i(p\rho - \frac{\pi}{4})} \right]. \quad (4)$$

The general normalizable solutions of Eq. (1) have the form

$$R_m(\rho) = c_m J_\mu(p\rho), \quad |m - \beta| > \sqrt{1 + \gamma^2}, \quad (5)$$

$$R_m(\rho) = a_m H_\mu^{(1)}(p\rho) + b_m H_\mu^{(2)}(p\rho), \quad \gamma < |m - \beta| < \sqrt{1 + \gamma^2}, \quad (6)$$

$$R_m(\rho) = a_m H_{i\mu}^{(1)}(p\rho) + b_m H_{i\mu}^{(2)}(p\rho), \quad |m - \beta| < \gamma \quad (7)$$

where  $\mu := |\nu|$  and  $J_\mu(x)$ ,  $H_\alpha^{(1,2)}(x)$  are the Bessel and Hankel functions with arbitrary coefficients  $a_m, b_m$ .

One can see that the normalizable wave functions can be singular at  $\rho = 0$  what is typical for singular potentials. This happens for small orbital momenta  $m$  when particles spend much time nearby the singular line  $\rho = 0$  and can fall onto it acquiring an infinite negative energy. Moreover, the linear independent solutions  $H_\alpha^{(1)}(p\rho)$  and  $H_\alpha^{(2)}(p\rho)$  are both square-integrable, and we have no criteria for selection of an unique solution to remove this ambiguity. In what followed we discuss different possible criteria for such choice.

### 3 The criteria for the selection of the unique solution

We consider now the possible criteria for fixing coefficients of Eqs. (6), (7). The behaviour of the solutions nearby the singularity  $\rho = 0$  will control this procedure. To expose what happens in general case we calculate the partial radial currents for the solutions (5) - (7). For Eq. (5) the partial radial currents are equal to zero. This means that the partial modes with  $|m - \beta| > \sqrt{1 + \gamma^2}$  are always scattered elastically. Using the properties of the Hankel functions we get for the remaining modes

$$j_m(\rho) = \frac{2}{\pi M \rho} (|a_m|^2 - |b_m|^2), \quad \gamma < |m - \beta| < \sqrt{1 + \gamma^2} \quad (8)$$

and

$$j_m(\rho) = \frac{2}{\pi M \rho} (|a_m|^2 e^{\pi\mu} - |b_m|^2 e^{-\pi\mu}), \quad |m - \beta| < \gamma. \quad (9)$$

The fact that the partial currents (8) and (9) through a cylindrical surface of a fixed radius  $\rho_0$ ,  $2\pi\rho_0 j_m(\rho_0)$  are independent on  $\rho_0$  means that the possible choice of the coefficients and the interpretation of the corresponding solutions have been connected with their behaviour at  $\rho \rightarrow 0$ .

These solutions have the following asymptotic behaviour at  $\rho \rightarrow 0$

$$R_m \rightarrow A_m \rho^{-\mu} + B_m \rho^\mu, \quad \gamma < |m - \beta| < \sqrt{1 + \gamma^2} \quad (10)$$

$$R_m(\rho) \rightarrow A_m \rho^{-i\mu} + B_m \rho^{i\mu}, \quad |m - \beta| < \gamma \quad (11)$$

where the coefficients  $A_m$  and  $B_m$  are connected with  $a_m$  and  $b_m$ . For the elastic scattering the ingoing and outgoing currents have to compensate to each other as this takes place for the modes of Eq. (5). This means that conditions  $|a_m| = |b_m|$  and  $|a_m| e^{\pi\mu/2} = |b_m| e^{-\pi\mu/2}$  must be fulfilled for Eq. (6) and Eq. (7), correspondingly. This leads to the following asymptotic behaviour of these solutions [16]

$$R_m(\rho) \rightarrow \rho^\mu + l_m \rho^{-\mu}, \quad l_m \in R_1 \quad (12)$$

and

$$R_m(\rho) \rightarrow \rho^{i\mu} + e^{i\vartheta_m} \rho^{-i\mu}, \quad 0 \leq \vartheta_m < 2\pi \quad (13)$$

that describe the elastic scattering without absorption. These asymptotic expressions show that the solution Eq. (7) contains at small  $\rho$  the ingoing and outgoing waves  $e^{\mp i\mu \ln \rho}$ , and the situation looks as if there exists an additional repulsive force or a reflective barrier with the support on  $\rho = 0$  which creates the outgoing wave. The self-adjoint extension procedure admits this interpretation. A rudiment of this phenomenon is present in Eq. (6).

Otherwise, if the conditions for the elastic scattering are not fulfilled, absorption of particles happens on the infinitely thin wire, and it was treated from different points of view in [12, 13, 15, 18]. The case of the total absorption has been also considered phenomenologically in [13, 14]. We notice that absorption can happen even in the pure AB case, see below.

An absorption criterion has been proposed in [6], and it has been used for the case of the attractive  $\rho^{-2}$  potential for  $\beta = 0$  in [7, 8]. The authors have eliminated the outgoing wave at  $\rho = 0$ , interpreting of the singularity  $\rho = 0$  as a sink. Taking  $b_m e^{-\pi\mu} = a_m e^{\pi\mu}$  in Eq. (7) and keeping only the ingoing wave  $e^{-i\mu \ln p\rho}$  in Eq. (11) at  $\rho \rightarrow 0$ , we obtain the solution [8]

$$R_m(\rho) = c_m J_{-i\mu}(p\rho), \quad |m - \beta| < \gamma \quad (14)$$

This solution has been used in [13, 15] to describe the inelastic scattering of neutral polarizable atoms from the charged wire placed in the uniform magnetic field.

In this case the partial absorption cross sections are equal to

$$\sigma_m^{\text{abs}} = \frac{1}{p} (1 - |S_m|^2) = \frac{1}{p} (1 - e^{-2\pi\mu}), \quad |m - \beta| < \gamma. \quad (15)$$

Now we come back to the radial solutions of Eq. (1) with arbitrary coefficients  $a_m$  and  $b_m$  and obtain the general expression for the partial absorption

cross sections. This permit us to work out analytically the case of the total absorption that has been considered phenomenologically in [13, 14].

Subtracting the radial function of the incoming plane wave, modified by the AB-phase factor [14], from the solutions (6, 7) we obtain the scattering amplitude (3) with the phase functions

$$S_m = e^{i\pi(m-\mu)}, \quad |m - \beta| > \sqrt{1 + \gamma^2}, \quad (16)$$

$$S_m = e^{i\pi(m-\mu)} \frac{a_m}{b_m}, \quad \gamma < |m - \beta| < \sqrt{1 + \gamma^2} \quad (17)$$

$$S_m = e^{i\pi m} e^{\pi\mu} \frac{a_m}{b_m}, \quad |m - \beta| < \gamma. \quad (18)$$

and the nonzero partial absorption cross sections

$$\sigma_m^{\text{abs}} = \frac{1}{p} \left( 1 - \frac{|a_m|^2}{|b_m|^2} \right), \quad \gamma < |m - \beta| < \sqrt{1 + \gamma^2} \quad (19)$$

$$\sigma_m^{\text{abs}} = \frac{1}{p} \left( 1 - e^{2\pi\mu} \frac{|a_m|^2}{|b_m|^2} \right), \quad |m - \beta| < \gamma. \quad (20)$$

For these orbital modes the partial absorption cross sections depend on the choice of the coefficients  $a_m$  and  $b_m$ . The different choice of these coefficients can be considered as the choice of different models of absorption.

We turn now to the approach to the absorption problem that has been proposed in [13, 14] for the case of the AB scattering polarizable atoms by a charge wire of a finite radius. The notion of an *absorption radius* was introduced there, such that incident particles with impact parameter  $a = |m - \beta|/p < \rho_{\text{abs}}$ , which refers to the kinetic angular momentum, will be absorbed. It determines an interval  $[-n_-, n_+]$  of the values of  $m$  inside of which the condition of the total absorption

$$S_m = 0, \quad -n_- < m < n_+ \quad (21)$$

was imposed instead of the value  $S_m = e^{i\pi m - \pi\mu}$  which followed from Eq. (18) at  $b_m e^{-\pi\mu} = a_m e^{\pi\mu}$ . This condition can be evidently derived analytically from Eq. (18) assuming that the coefficient  $a_m = 0$  if *the absorption radius* less than *the critical radius* defined by the values of  $m$  for which  $\nu^2 < 0$ . The corresponding radial solution is the Hankel function

$$R_m(\rho) = \frac{1}{2} e^{i\pi m} e^{\pi\mu/2} H_{i\mu}^{(2)}(p\rho) \quad (22)$$

which has the asymptotic behavior at  $\rho \rightarrow \infty$  like Eq. (4) with  $S_m = 0$ . At small  $\rho$  it contains both the ingoing and outgoing waves, moreover, the outgoing wave is weakened so to escape at infinity. In this case the partial scattering amplitudes are equal to

$$f_m = -\frac{e^{-i\frac{\pi}{4}}}{p} \cos \pi\beta, \quad |m - \beta| < \gamma,$$

and the partial absorption cross sections are equal to their maximal values

$$\sigma_m^{\text{abs}} = \frac{1}{p}, \quad |m - \beta| < \gamma.$$

For the intermediate case of Eq. (17) the condition of the total absorption  $S_m = 0$  is realized if  $a_m = 0$ . Then the corresponding wave function reads

$$R_m(\rho) = \frac{1}{2} e^{i\pi m} e^{-i\pi\mu/2} H_\mu^{(2)}(p\rho). \quad (23)$$

We note that absorption can happens for the pure AB scattering when the attractive potential is absent ( $\gamma = 0$ ). Then, for the partial modes with  $|m - \beta| < 1$ . i.e. for the values of  $m = 0$  and  $m = 1$ , it is possible to get any value of the partial absorption cross sections up to its maximal value  $1/p$ . For the pure attractive potential ( $\beta = 0$ ) the number of modes that can be absorbed,  $|m| < \gamma$ , depends on the value of  $\gamma$ .

## 4 Other singular attractive potentials

We consider now the Schrödinger equation Eq. (1) with the more singular attractive potential

$$U(\rho) = -\frac{\kappa^2}{\rho^4}. \quad (24)$$

The Schrödinger equation with this potential alone describes the scattering of ions by polarization forces [6]. We keep the AB potential in addition to the potential (24). Then the radial equation takes the form

$$R_m''(\rho) + \frac{1}{\rho} R_m'(\rho) \frac{(m - \beta)^2}{\rho^2} R_m(\rho) + \frac{\lambda^2}{\rho^4} R_m(\rho) + p^2 R_m(\rho) = 0 \quad (25)$$

and by the substitution  $\rho = \rho_0 e^x$ ,  $\rho_0 := \sqrt{\lambda/p}$  can be reduced to the Mathieu equation of imaginary argument

$$R_m''(x) - (a - 2q \cosh 2x) R_m(x) = 0 \quad (26)$$

with the parameters  $a := (m - \beta)^2$  and  $q := p\lambda$ .

Asymptotic behaviour of solutions of Eq. (26) at large  $\rho$  (large positive  $x$ ) is well known,

$$R_m^{(1,2)}(\rho) \sim H_{m-\beta}^{(1,2)}(p\rho) \sim \sqrt{\frac{2}{\pi p \rho}} e^{\pm i(p\rho - \frac{\pi}{2}|m-\beta| - \frac{\pi}{4})}, \quad \rho \rightarrow \infty. \quad (27)$$

The Mathieu functions Eq. (27) form a complete set and the total solution of Eq. (25) can be represented by their linear combination [19]

$$R_m(\rho) = a_m R_m^{(1)}(\rho_0) + b_m R_m^{(1)}(\rho_0). \quad (28)$$

With these radial functions we obtain the following expression for the phase function of Eq. (4)

$$S_m = e^{i\pi(m-|m-\beta|)} \frac{a_m}{b_m}. \quad (29)$$

Now we can choose the coefficients  $a_m$  and  $b_m$  in accordance with the different criteria discussed above. For this aim we have to consider the asymptotic behaviour of solutions of Eq. (26) at small  $\rho$  (large negative  $x$ ). There are two other Mathieu functions which describe the ingoing and outgoing waves nearby the singularity line  $\rho = 0$ ,

$$R_m^{(3,4)}(\rho) \sim H_{m-\beta}^{(1,2)}\left(\frac{\lambda}{\rho}\right) \sim \sqrt{\frac{2\rho}{\pi\lambda}} e^{\pm i(\frac{\lambda}{\rho} - \frac{\pi}{2}|m-\beta| - \frac{\pi}{4})}, \quad \rho \rightarrow 0 \quad (30)$$

which also form a complete set. Now, to work out the elastic scattering, we have to impose the self-adjointness condition on the Hamiltonian of Eq. (25) [5], taking the linear combination

$$R_m^{(\text{el})}(\rho) = e^{-i\theta_m} R_m^{(3)}(\rho) + e^{i\theta_m} R_m^{(4)}(\rho). \quad (31)$$

Using their connections with the Mathieu functions  $R_m^{(1,2)}(\rho)$  we obtain the coefficients  $a_m$  and  $b_m$  and the phase function (29) of the elastic scattering. On contrary, eliminating of the outgoing wave at  $\rho = 0$  to describe absorption we have to connect the solution  $R_m^{(3)}(\rho)$  with the Mathieu functions  $R_m^{(1,2)}(\rho)$  to find another coefficients  $a_m$  and  $b_m$ . In this way the inelastic scattering of ions by polarization forces has been considered and the capture cross section has been evaluated in [6]. At least, to get the total absorption of given modes we have to put zero the corresponding coefficients  $a_m$ .

The choice of the coefficients  $a_m$  and  $b_m$  depends on model of absorption under consideration. For example, one can put  $S_m = S_m^{\text{el}}$  for large  $|m| \geq$

$m_{\text{abs}}$  (large impact parameters) and  $S_m = 0$  for  $|m| \leq m_{\text{abs}}$  or to consider a intermediate regime from the elastic scattering to the total absorption.

Up to now we dealt with potentials that are singular on the line. The similar results can be obtained for potentials with singularities on a surface. For example, one can use the potential that is singular on the cylindric surface  $\rho = \rho_0$ ,

$$U(\rho) = -\kappa \frac{e^{-|\rho-\rho_0|/l}}{(\rho - \rho_0)^n} \quad n \geq 2$$

which will imitate absorption in a thin layer of width  $\sim l$  nearby this surface. Of cause, the analytical calculations in this case are very cumbersome, if possible.

## 5 Conclusion

The main result of the paper is following: If partial wave functions of a quantum mechanical problem are not fixed by the normalization conditions as this happens in the presence of singular potentials, then the corresponding arbitrariness can be used to describe not only elastic scattering but also inelastic one (absorption). By different choice of partial radial wave functions various models of absorption can be realized, beginning from almost elastic scattering till maximal possible values of partial absorption coefficients.

We give up unsolved very important problem what type of physical situations with regular potentials corresponds in a singular limit to different choice of the partial wave functions describing elastic scattering or absorption.

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